

# Temperature measurement from perturbations

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## Abstract

The concept of the configuration temperature is extended to discrete or discontinuous systems through the identification of the temperature as the nontrivial root of several integral equations regarding the distribution of the energy change upon configuration perturbations.

Temperature is traditionally computed from the kinetic energy; but more recent studies [1-3] showed that it can be also measured from derivatives of the potential energy  $U(\mathbf{q})$  with respect to coordinates  $\mathbf{q}$ : the reciprocal temperature  $\beta = 1/(k_B T)$  (with  $k_B$  and  $T$  being the Boltzmann constant and absolute temperature, respectively) satisfies

$$\beta = \left\langle \nabla \cdot \left[ \frac{\nabla U(\mathbf{q})}{\nabla U(\mathbf{q}) \cdot \nabla U(\mathbf{q})} \right] \right\rangle \approx \frac{\langle \nabla^2 U(\mathbf{q}) \rangle}{\langle \nabla U(\mathbf{q}) \cdot \nabla U(\mathbf{q}) \rangle}, \quad (1)$$

where “ $\langle \dots \rangle$ ” denotes an ensemble average, and  $\beta$  takes the respective meaning in different ensembles, e.g., it is the logarithmic derivative of the density of states  $g(E)$  in the microcanonical ensemble [i.e.,  $\beta(E) = \frac{\partial}{\partial E} \log g(E)$  [4, 5]], or the parameter in the canonical one. Eq. (1) is exact in the canonical ensemble [3, 5], but generally approximate, with an error of order  $1/N$  in a system of  $N$  degrees of freedom [2, 3].

Eq. (1) allows us to compute the temperature from a set of configurations without the knowledge of the velocities. This *configuration temperature* has found applications in, e.g., verifying a Monte Carlo simulation [2], entropic sampling [6], constructing a thermostat [7], free-energy calculation [8], etc.

However, Eq. (1) requires a continuous system with up to the second derivatives of the potential energy; but the computation of second derivatives is often demanding, and the molecular potential is sometimes discontinuous by tail truncation [2, 9, 10] or simply discrete [9], making the formulas inapplicable. We will show below that the evaluation of derivatives can be replaced by that of the potential-energy change under a random perturbation, giving rise to more convenient expressions of the temperature.

Given a configuration  $\mathbf{q}$ , a small perturbation  $\mathbf{u}$  in coordinates changes the potential energy by  $\varepsilon = U(\mathbf{q} + \mathbf{u}) - U(\mathbf{q}) \approx \nabla U \cdot \mathbf{u} + \frac{1}{2} \mathbf{u} \cdot \nabla \nabla U \cdot \mathbf{u}$ . Now consider a random

$\mathbf{u}$ , whose distribution is symmetric such that the probabilities of  $\mathbf{u}$  and  $-\mathbf{u}$  are equal, and component-independent such that  $\overline{u_i u_j} = \sigma^2 \delta_{ij}$  (where the overline denotes an average over the perturbation  $\mathbf{u}$ , and  $\sigma$  is the standard deviation of any  $u_i$ ); then on average, we have, (i)  $\overline{\varepsilon} \approx \frac{1}{2} \overline{\mathbf{u} \cdot \nabla \nabla U \cdot \mathbf{u}} = \frac{1}{2} \nabla^2 U \sigma^2$ , and (ii)  $\overline{\varepsilon^2} \approx \overline{(\nabla U \cdot \mathbf{u})^2} = (\nabla U \cdot \nabla U) \sigma^2$  to the leading order. We now take the ensemble averages over  $\mathbf{q}$  (denoted by “ $\langle \dots \rangle$ ”, not to be confused with the overline) of the two; and their ratio is

$$\lim_{\sigma \rightarrow 0} \frac{2 \langle \overline{\varepsilon} \rangle}{\langle \overline{\varepsilon^2} \rangle} = \frac{\langle \nabla^2 U \rangle}{\langle \nabla U \cdot \nabla U \rangle} \approx \beta. \quad (2)$$

The last step follows from Eq. (1) (in fact, we have  $\lim_{\sigma \rightarrow 0} 2 \langle \overline{\varepsilon^k} \rangle / \langle \overline{\varepsilon^{k+1}} \rangle \approx \beta$  for any odd positive integer  $k$ ). It shows an asymmetry  $\langle \overline{\varepsilon} \rangle > 0$  (since  $\beta$  is usually positive), even though the perturbation is symmetric; this is because a potential-energy surface usually on average adopts a convex shape, which favors a positive  $\varepsilon$  instead of a negative one [see Fig. 1(a)].

Eq. (2) is a “literal” translation of Eq. (1) in terms of a random perturbation; but it no longer requires derivatives of the potential energy function  $U(\mathbf{q})$ , and can thus be applied to some discrete  $U(\mathbf{q})$ . Nonetheless, the perturbation still needs to be small, for it is derived from the first two moments of the distribution of  $\varepsilon$ . The following integral relations use all moments of the distribution, and thus allow larger perturbations.

First consider a simple case for the canonical ensemble. If each configuration  $\mathbf{q}$  is shifted by  $\mathbf{u}$  to  $\mathbf{q}' = \mathbf{q} + \mathbf{u}$ , and the potential-energy change  $\varepsilon = U(\mathbf{q}') - U(\mathbf{q})$ , then [11]

$$\langle \exp(-\beta \varepsilon) \rangle_\beta = 1, \quad (3)$$

because

$$\langle \exp(-\beta \varepsilon) \rangle_\beta = \int \exp(-\beta \varepsilon) \frac{\exp[-\beta U(\mathbf{q})]}{Z(\beta)} d\mathbf{q} = \int \frac{\exp[-\beta U(\mathbf{q}')] }{Z(\beta)} d\mathbf{q}' = 1,$$

where  $Z(\beta) \equiv \int e^{-\beta U(\mathbf{q})} d\mathbf{q}$  is the configuration partition function, and  $\frac{\exp[-\beta U(\mathbf{q})]}{Z(\beta)}$  is the normalized weight for configuration  $\mathbf{q}$ .

Like Eq. (2), Eq. (3) determines  $\beta$  entirely from the statistical moments of  $\varepsilon$ :

$\sum_{n=0}^{\infty} (-\beta)^n \langle \varepsilon^n \rangle_\beta / n! = 1$ ; but it does so as an implicit equation. We can, however, obtain an explicit expression for  $\beta$  if the distribution of  $\varepsilon$  is narrow or Gaussian:

$$0 = \log \langle \exp(-\beta \varepsilon) \rangle_\beta \approx -\beta \langle \varepsilon \rangle_\beta + \frac{1}{2} \beta^2 \langle \Delta \varepsilon^2 \rangle_\beta,$$

where  $\Delta \varepsilon = \varepsilon - \langle \varepsilon \rangle_\beta$ . The only solution, apart from  $\beta = 0$ , is

$$\beta \approx 2 \langle \varepsilon \rangle_\beta / \langle \Delta \varepsilon^2 \rangle_\beta. \quad (3')$$

Eq. (3') differs from (2) by using  $\Delta \varepsilon$  instead of  $\varepsilon$  on the denominator; but since  $\overline{\langle \varepsilon \rangle}_\beta$

(the perturbation-averaged  $\langle \varepsilon \rangle_\beta$ ) and  $\varepsilon$  are  $O(\sigma^2)$  and  $O(\sigma)$ , respectively, the

difference is trifle for a small  $\sigma$ . Thus, Eq. (3) can be considered as a generalization of Eq. (2) for larger perturbations.

We will extend Eq. (3) to a few other ensembles below. We first show that it approximately applies to the temperature of potential energy  $\beta_U(U) \equiv \frac{d}{dU} \log g_U(U)$ ,

where  $g_U(U) \equiv \int \delta(U(\mathbf{q}) - U) d\mathbf{q}$  is the density of configurations of the same potential energy  $U$ :

$$\langle \exp[-\beta_U(U) \varepsilon] \rangle_U \approx 1. \quad (4)$$

We assume that the perturbation  $\mathbf{u}$  has a symmetric distribution, such that  $\mathbf{u}$  and  $-\mathbf{u}$  are equally likely. Then, there is a microscopically reversibility: for a  $\mathbf{u}$  that carries  $\mathbf{q}$  to  $\mathbf{q}'$ , the reverse  $-\mathbf{u}$  that carries  $\mathbf{q}'$  back to  $\mathbf{q}$  shares the same probability. It follows that the flow  $\Phi(U, U + \varepsilon)$ , or the number of  $\mathbf{u}$  that reach the  $U + \varepsilon$  state from the  $U$  state (which is defined as all configurations with the potential energy being  $U$ ), equals the reverse flow  $\Phi(U + \varepsilon, U)$  [see Fig. 1(b)]:

$$\Phi(U, U + \varepsilon) = \Phi(U + \varepsilon, U). \quad (5)$$

But the ratio of  $\Phi(U, U + \varepsilon)$  to  $g_U(U)$  is just  $p_U(\varepsilon)$ , the distribution of energy change  $\varepsilon$  of the perturbations started from the  $U$  state; so

$$p_U(\varepsilon) = \Phi(U, U + \varepsilon) / g_U(U).$$

It is reasonable to assume that  $p_U(\varepsilon)$  changes slowly with  $U$  such that

$$p_U(\varepsilon) \approx p_{U-\varepsilon}(\varepsilon). \quad (6)$$

Thus,

$$\frac{p_U(-\varepsilon)}{p_U(+\varepsilon)} = \frac{\Phi(U, U - \varepsilon)}{\Phi(U, U + \varepsilon)} = \frac{\Phi(U - \varepsilon, U)}{\Phi(U, U + \varepsilon)} \approx \frac{g_U(U - \varepsilon)}{g_U(U)} \approx \exp[-\beta_U(U) \varepsilon], \quad (7)$$

where we have used Eq. (5) in the second step, and Eq. (6) in the third. Finally,

$$\langle \exp(-\beta_U \varepsilon) \rangle_U = \int_{-\infty}^{+\infty} \exp(-\beta_U \varepsilon) p_U(\varepsilon) d\varepsilon \approx \int_{-\infty}^{+\infty} p_U(-\varepsilon) d\varepsilon = 1,$$

[see Fig. 1(c)]. This completes the argument. It also shows that Eq. (4) holds for a limited (and renormalized) portion of the distribution in  $(-\varepsilon_{\max}, \varepsilon_{\max})$  (thus, we can drop large  $\varepsilon$  commonly caused by clashes in perturbed configurations in a molecular system).

Eq. (7) is stronger than Eq. (4), for it applies to *any*  $\varepsilon$ ; geometrically it means that the regions A and B in Fig. 1(b) are roughly congruent. Thus, there are a few additional integral relations, e.g.,

$$\langle \varepsilon^k \min\{1, \exp[-\beta_U(U) \varepsilon]\} \rangle_U \approx 0, \quad (8)$$

for an odd  $k$ . Since  $\min\{1, \exp(-\beta\varepsilon)\}$  is the Metropolis acceptance probability [10, 12, 13], Eq. (8) ( $k=1$ ) means that the energy change after a Metropolis step starting from the  $U$  state averages to zero if the parameter  $\beta$  matches  $\beta_U(U)$ . Similarly, at the midpoint  $\beta_h = \frac{1}{2} \beta_U(U)$ , the function  $\exp(-\beta_h \varepsilon) p_U(\varepsilon)$  is also even; so

$$\langle \varepsilon^k \exp[-\frac{1}{2} \beta_U(U) \varepsilon] \rangle_U \approx 0, \quad (9)$$

with an odd integer  $k$ . In both cases, the  $\varepsilon^k$  can be replaced by an arbitrary odd function  $f_{\text{odd}}(\varepsilon)$ .

The above relations can be extended to the canonical/microcanonical ensemble, or more generally, one that is composed of constant- $U$  ensembles. In this case, we have

$1 = \int g_U(U) w(U) dU$ , where  $w(U)$  is the normalized weight of a configuration [which is  $e^{-\beta U} / Z(\beta)$  for the canonical ensemble, or  $(E - U)^{N/2-1} / g(E)$  for the microcanonical one [6], with  $g(E)$  being the density of states]. The distribution  $p_w(\varepsilon)$  in this ensemble is

$$p_w(\varepsilon) = \langle p_U(\varepsilon) \rangle_w = \int \Phi(U, U + \varepsilon) w(U) dU,$$

where  $\langle \dots \rangle_w$  denotes an average in this ensemble. Eq. (7) becomes

$$\frac{p_w(-\varepsilon)}{p_w(+\varepsilon)} = \frac{\langle p_U(\varepsilon) w(U + \varepsilon) / w(U) \rangle_w}{\langle p_U(\varepsilon) \rangle_w} \approx \langle \exp[-\beta_w(U) \varepsilon] \rangle_w \approx \exp[-\langle \beta_w(U) \rangle_w \varepsilon],$$

where  $\beta_w(U) \equiv -\frac{\partial}{\partial U} \log w(U)$ , and we have approximated  $w(U + \varepsilon)/w(U)$  by  $\exp[-\beta_w(U)\varepsilon]$ , and ignored its correlation with  $p_U(\varepsilon)$ . Thus, Eqs. (4), (8) and (9), when used in this ensemble, give the temperature defined as  $\langle \beta_w(U) \rangle_w = \langle -\frac{\partial}{\partial U} \log w(U) \rangle_w$ , which is  $\beta$  in the canonical ensemble, or  $\beta(E) = \langle \frac{N/2-1}{E-U} \rangle_E$  in the microcanonical one.

Eqs. (4) and (7) resemble the Jarzynski equality [14] and fluctuation theorems [15]; but they are *not* identities in general, for the temperature determined here matches the logarithmic derivative of the flow  $\Phi(U, U + \varepsilon)$ , instead of that of  $g_U(U)$ , and thus has an  $O(1/N)$  error. Besides, although the integral relations allow larger perturbations than Eqs. (2) and (3'),  $\varepsilon$  should still be small in the thermodynamic sense that  $\beta_U(U)$  does not change too much from  $U$  to  $U + \varepsilon$ . Eq. (7) also resembles the detailed balance condition used in the broad-histogram simulation [16]; but it was further approximated by Eq. (6) to allow an integral form, which avoids direct handling of the distribution.

We use Eqs. (2)-(4), (8) and (9) in a molecular dynamics [9, 10] (MD) or Monte Carlo [9, 10, 12] (MC) simulation in this way: once every few trajectory frames, we perturb the current configuration  $\mathbf{q}$  by a random  $\mathbf{u}$ , and register the resulting change  $\varepsilon = U(\mathbf{q} + \mathbf{u}) - U(\mathbf{q})$  in the potential energy; the formulas then estimate the temperature  $\beta$  from the accumulated distribution  $p(\varepsilon)$ . Since no derivative of  $U(\mathbf{q})$  is needed, they apply to systems with discrete or discontinuous potentials; we may further allow discrete configurations  $\mathbf{q}$  and perturbations  $\mathbf{u}$ , e.g., in the Ising model,  $\mathbf{q}$  is a discrete spin configuration, and  $+\mathbf{u}$  means to flip a random spin.

We now discuss some numerical results. Four  $\varepsilon$ -distributions  $p(\varepsilon)$  from independent simulations on the 108-particle Lennard-Jones (LJ) fluid at  $\rho = 0.7$  and

$\beta_0 = 1.0$  are shown in Fig. 2(a). Except the first simulation, which used a regular MD (corresponding to a microcanonical-like ensemble), all simulations used the Metropolis algorithm (corresponding to the canonical ensemble) to generate trajectories. To avoid artifacts from the potential truncation, the pair potential was switched smoothly from the standard form  $u(r) = 4(r^{-12} - r^{-6})$  at  $r_s = 2.0$  to a 7th polynomial till  $r_c = 2.5$ , at which the polynomial and first three derivatives vanished [17]. In the first three cases, the perturbation applied to a random particle, and the Cartesian coordinates are displaced by random numbers within  $(-u_{\max}, u_{\max})$ , with  $u_{\max} = 0.05$  (the first two cases) or 0.1 (the third); but in the last case, it applied to all particles in the system with  $u_{\max} = 0.01$ . The number of perturbations was  $10^7$  in each case. A comparison of the first two cases shows that the distribution depended little on whether the ensemble was microcanonical-like (MD) or canonical (MC). A comparison of the second and third cases shows that the amplitude of the single-particle perturbation mainly adjusted the aspect ratio of the distribution, but retained the generic shape, which peaked at  $\varepsilon = 0$ . The distribution from the all-particle perturbation, however, adopted a different Gaussian-like shape. Despite the variety, the integral relations applied to all cases, e.g., the  $\beta$  given by Eq. (4) were 1.0077, 0.9990, 1.0160, and 0.9997, respectively.

The solution process of Eq. (3) is illustrated in Fig. 2(b): we plotted  $\langle \exp(-\beta\varepsilon) \rangle$  against  $\beta$ , and its intersection with 1.0 gave the required temperature. Three systems, the LJ fluid (with both single- and all-particle perturbations), 108-particle square-well [9] fluid and  $32 \times 32$  Ising model were simulated in the canonical ensemble at  $\beta_0 = 1.0$  using the Metropolis algorithm. The number of perturbations was  $10^7$  in each case, and the



computed  $\beta$  were 1.0160 (LJ, single), 0.9997 (LJ, all), 1.0003 (square-well), and 1.0004 (Ising), respectively. The first two simulations on the LJ fluid were the same as the last two in Fig. 2(a). The square-well fluid differed from the LJ fluid by using a discrete pair potential, which is infinity if the particle distance  $r < r_a$ , or  $-1$  if  $r_a \leq r < r_b$ , or 0 otherwise (here  $r_a = 1$  and  $r_b = 1.5$ ); the perturbation was a single-atom displacement with  $u_{\max} = 0.1$ ;  $\rho = 0.7$ ; perturbations that produced clashes, hence infinite  $\varepsilon$ , were excluded from entering Eq. (3), for clashed configurations contribute nothing to the partition function. The perturbation in the Ising model was a flip of a random site.

In Fig. 2(c), the temperatures computed from Eqs. (1)-(3), (8) and (9) ( $k = 1$  in the last two cases), after averaged over  $10^7$  repeats, were plotted against  $u_{\max}$ , the size of the single-particle perturbation. All formulas worked well with a small  $u_{\max}$ , but with a large  $u_{\max}$ , Eq. (2) and (3') quickly lost accuracy [Eq. (3') would, however, perform much better for the all-particle perturbation, whose distribution  $p(\varepsilon)$  was Gaussian-like], while the integral formulas were little affected.

The effect of the potential truncation [2] was studied using a set of MC simulations ( $10^7$  single-particle perturbations in each,  $u_{\max} = 0.05$ ) with the LJ potential deliberately truncated at various  $r_c$ . The discontinuity rendered Eq. (1) approximate; and as shown in Fig. 2(d), Eq. (1) was indeed affected by a small  $r_c$ , while Eqs. (3), (8), and (9) were not.

The temperature  $\beta_U(U)$  of the potential energy was computed on the  $32 \times 32$  Ising model. To cover the entire energy range, an entropic sampling [6, 18] simulation was run using the exact density of states  $g_U^*(U)$  [19] in the sampling weight for  $10^7$  MC steps per

site. As shown in Fig. 3, the temperature from Eqs. (2) and (3') behaved badly except around  $U \approx 0$  or  $\beta_U \approx 0$ , while Eqs. (4), (8) and (9) showed good agreement with the reference, computed as  $\beta_U^*(U) = \frac{\partial}{\partial U} \log g_U^*(U)$ . This is expected, as the smallest energy change is 4 in this case, the condition  $\beta\varepsilon \ll 1$  is hard to meet, while  $\varepsilon$  is still smaller than the energy fluctuation to justify the use of the integral relations. But even in the latter case, there was an  $O(1)$  difference between the logarithm density of states from the integral  $\log g_U(U) = \int_0^U \beta_U(U') dU'$  and the exact  $\log g_U^*(U)$  (see the inset of Fig. 3), which means that the temperature from the integral relations has an  $O(1/N)$  systematic error [as the entire potential-energy range is  $O(N)$ ].

As an application, Eq. (3) can be used to efficiently match two potential energy functions, so that a simplified or coarse-grained function can emulate a more complex or realistic one. We use the following fluid example as a proof of principle. The aim was to make the configurations produced by the square-well potential  $U_{\text{sq}}(\mathbf{q})$  similar to those by the LJ potential  $U_{\text{LJ}}(\mathbf{q})$  under  $\rho = 0.7$ ,  $\beta = 1.0$ . To do this, we first ran a simulation using  $U_{\text{sq}}(\mathbf{q})$  as the potential energy, and then evaluated, from configurations of the trajectory, the effective temperature  $\beta_{\text{LJ}}$  by Eq. (3) with the single-particle perturbation ( $u_{\text{max}} = 0.1$ ) and  $U(\mathbf{q}) = U_{\text{LJ}}(\mathbf{q})$ ; we repeat the process with a different parameter  $r_a$  in  $U_{\text{sq}}(\mathbf{q})$  ( $r_b$  is kept at 1.5 for simplicity) until  $\beta_{\text{LJ}}$  matches  $\beta$ . After  $r_a$  was shifted from 1.0 to 0.9657,  $\beta_{\text{LJ}}$  changed from 1.865 to 0.999; as a result  $\langle U_{\text{LJ}}/N \rangle$  was changed from  $-5.289$  to  $-4.822$ , which was much closer to the reference  $-4.887$  [20], although we did not explicitly matched the energy [we must expect a small deviation, for the method is

approximate: the configurations generated by  $U_{\text{sq}}(\mathbf{q})$  and  $U_{\text{LJ}}(\mathbf{q})$  can be entirely different in principle]. The procedure was economical for the energy change needed by Eq. (3) can be evaluated locally; in contrast, had we matched the potential energy instead of temperature, it would involve a global evaluation, as well as a second simulation using  $U_{\text{LJ}}(\mathbf{q})$  as the potential energy to compare the averages  $\langle U_{\text{LJ}} \rangle$  in the two cases.

To sum up, temperature  $\beta$  can be extracted from the distribution  $p(\varepsilon)$  of the potential-energy change  $\varepsilon$  caused by configuration perturbations, as the nontrivial root of Eqs. (4), (8) or (9). If the perturbation or  $\beta$  is small, simpler formulas, such as Eqs. (2) and (3'), also apply. Finally, we can generalize the formulas for an arbitrary distribution  $\rho(X)$  of  $X = X(\mathbf{q})$  [17], e.g., Eq. (4) reads

$$\left\langle \exp\left[-\frac{d}{dX} \log \rho(X) \Delta X^*\right] \right\rangle_X \approx 1,$$

where  $\Delta X^*$  is the change of  $X$  after a MC/MD step (note,  $\Delta X^* = 0$  for a failed MC trial), and  $\langle \dots \rangle_X$  denotes a configuration average at a fixed  $X$  in the simulation ensemble [this follows from the mapping:  $g_U(U) \rightarrow \rho(X)$ ,  $\beta_U(U) \rightarrow \frac{d}{dX} \log \rho(X)$ ].

The computer code of the examples can be found in <http://simulalgo.appspot.com/rpt>.

## Figure Captions

Figure 1. (a) The intersection of the sphere (dotted) of perturbations  $\mathbf{u}$  (isotropic, fixed length) with the constant- $U$  surface at  $U + \varepsilon$  has a larger circumference than that with the constant- $U$  surface at  $U - \varepsilon$ ; thus  $+\varepsilon$  occurs more often than  $-\varepsilon$ , even for a symmetric  $\mathbf{u}$ . (b) The forward and reverse flows (arrows), e.g.,  $\Phi(U, U + \varepsilon)$  and  $\Phi(U + \varepsilon, U)$ , are balanced between any two macroscopic constant- $U$  ensembles (ovals); and the flow  $\Phi(U, U + \varepsilon)$  is proportional to the ensemble population  $g_U(U)$ . (c) The distribution  $p_U(\varepsilon)$  (solid line) of the energy-change  $\varepsilon$  upon perturbations. With the correct  $\beta$ ,  $\exp(-\beta\varepsilon)p_U(\varepsilon)$  (dashed) coincides with the horizontal reflection  $p_U(-\varepsilon)$  of  $p_U(\varepsilon)$ , and thus satisfies  $\langle \exp(-\beta\varepsilon) \rangle_U = 1$ ; it is not so with another  $\beta'$  (dot-dashed).

Figure 2. (a) The distributions of the potential-energy change  $\varepsilon$ . (b) The intersection of  $\langle \exp(-\beta\varepsilon) \rangle$  and 1.0 gives the correct  $\beta$ . (c) The temperature versus the perturbation amplitude  $u_{\max}$ . (d) The temperature versus the potential truncation  $r_c$ .

Figure 3. The profile of the temperature of potential energy  $\beta_U(U)$  along  $U$  in the  $32 \times 32$  Ising model. Inset: the error of  $\log g_U(U) = \int_0^U \beta_U(U') dU'$ .

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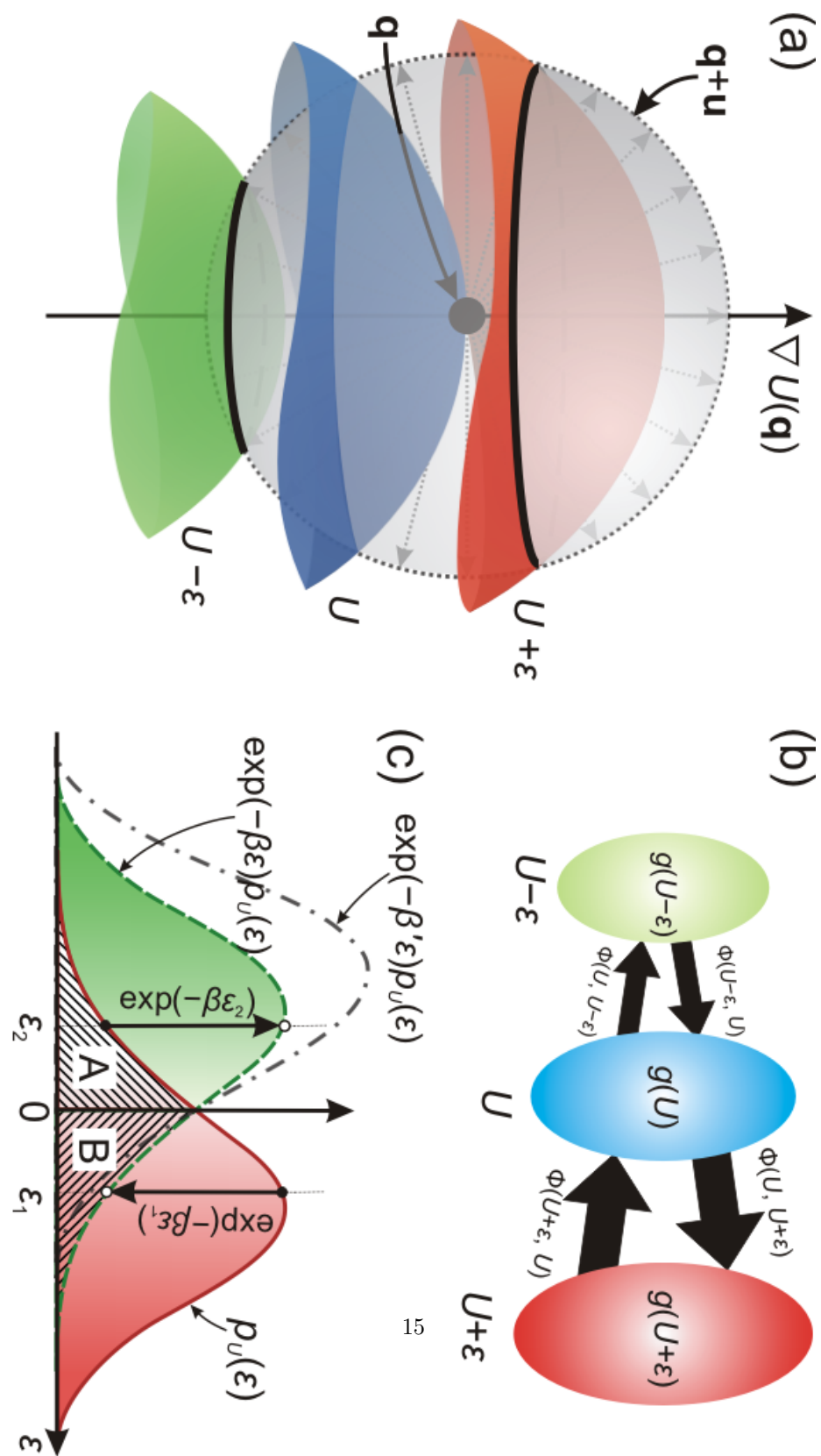


Figure 1:

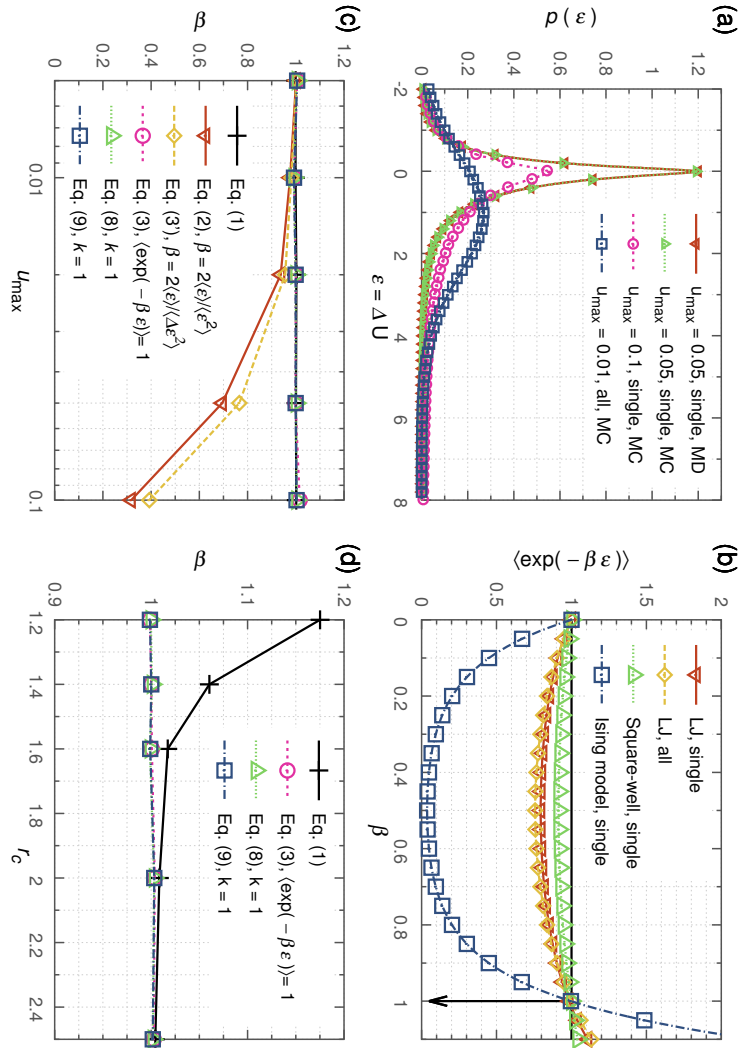


Figure 2:



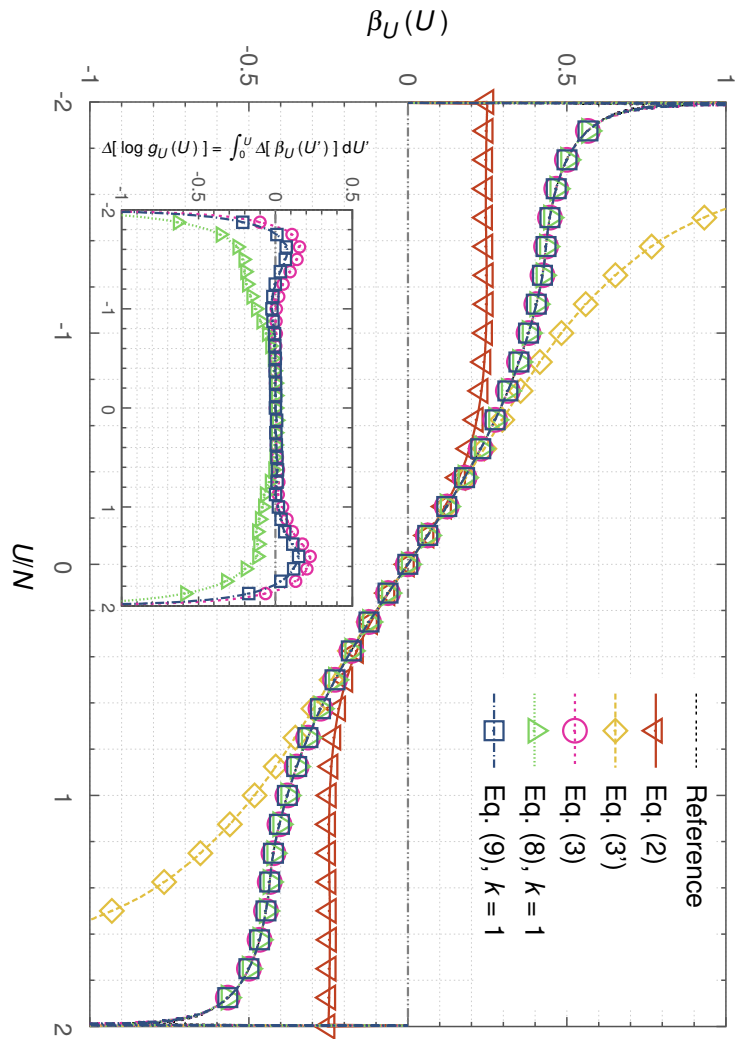


Figure 3: